

Universal magnetic excitation spectrum in cuprates

J. M. Tranquada,^a H. Woo,^{a,b} T. G. Perring,^b H. Goka,^c G. D. Gu,^a G. Xu,^a M. Fujita,^c
and K. Yamada^c

^a*Physics Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*

^b*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK*

^c*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

Abstract

We have recently used inelastic neutron scattering to measure the magnetic excitation spectrum of $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$ up to 200 meV. This particular cuprate is of interest because it exhibits static charge and spin stripe order. The observed spectrum is remarkably similar to that found in superconducting $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$; the main differences are associated with the spin gap. We suggest that essentially all observed features of the magnetic scattering from cuprate superconductors can be described by a universal magnetic excitation spectrum multiplied by a spin gap function with a material-dependent spin-gap energy.

Key words: magnetic excitations, neutron scattering, cuprates, stripes

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1. Introduction

Given the prominent role of antiferromagnetism in the typical phase diagram for cuprate superconductors, it is commonly believed that antiferromagnetic spin fluctuations play a significant role in the mechanism of superconductivity. Experimentally, however, it has been difficult to establish a universal trend for the magnetic excitations that applies across all hole-doped cuprate families.

One fairly broad experimental trend involves the appearance of a magnetic “resonance” peak at roughly 40 meV in the superconducting state. Centered at the antiferromagnetic wave vector \mathbf{Q}_{AF} , this feature has been observed in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ [1,2], $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ [3], and $\text{Tl}_2\text{Ba}_2\text{CuO}_6$ [3,4]. A problem with this trend is that an analo-

gous feature has not been observed in the family of cuprates associated with $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

Our recent neutron scattering results for $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$ (LBCO) [5] allow one, for the first time, to identify a universal magnetic excitation spectrum for the cuprates. As we discuss below, the observed excitations show dispersions quite similar to those found in several recent studies of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) [6,7,8,9]. The major difference is with respect to the temperature and frequency dependence associated with the spin gap. We note that the temperature-dependent effects in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) are associated with a small spin gap, and thus occur at an energy scale where the magnetic excitations are incommensurate [10,11,12,13,14]. We suggest that all of the observed behavior can be described by a

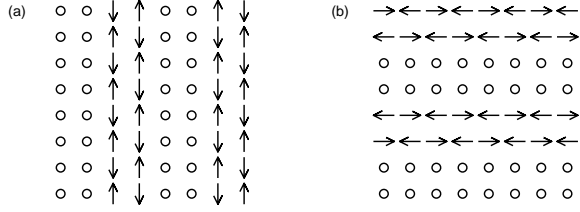


Fig. 1. Cartoons of charge and spin stripes, showing two types of stripe domain. Arrows indicate Cu spins; circles indicated hole-rich regions.

single phenomenological model in which there is a universal magnetic excitation spectrum with the intensity multiplied by a gap function, with the spin gap energy roughly correlated with the superconducting transition temperature, T_c , and varying among cuprate families.

Another significant feature of our LBCO sample is that it exhibits static charge and spin stripe order [15]. Cartoons of the two possible stripe domains are shown in Fig. 1. The stripe order competes with superconductivity [16], so that the T_c of our sample is less than 6 K, well below the measurement temperature of 12 K. As our measurements are in the normal state, they indicate that the universal features of the excitation spectrum cannot depend on the existence of a coherent superconducting state. We discuss interpretations of the spectrum in terms of the quantum excitations of finite spin clusters such as 2-leg antiferromagnetic ladders. We also comment on alternative explanations in terms of fermiology.

2. Neutron scattering experiment on $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$

Neutron scattering measurements have established that stripe order appears in LBCO below 50 K [15]. For the present experiment, four large crystals (each 8 mm $\phi \times 50$ mm) with a total mass of 58 g were grown at Brookhaven. After coaligning the crystals at the JRR-3M reactor in Tokai, Japan, the sample was transported to the ISIS spallation source. The experiment was performed on the MAPS spectrometer, a direct-geometry time-of-flight spectrometer with a large position-sensitive

area detector. The sample was aligned with the c axis parallel to the incident beam direction. Measurements were performed with incident energies of 80, 240, and 500 meV.

The results have been reported in Ref. [5]. At low energies (≤ 10 meV), we observe magnetic excitations peaked at the wave vectors of the magnetic superlattice peaks [15]. These are essentially the same incommensurate wave vectors at which the low-energy magnetic excitations are found in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [17]. With increasing energy, the excitations disperse inwards towards \mathbf{Q}_{AF} , with no obvious outwardly dispersing excitations; similar results have recently been reported for optimally-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [14]. These excitations merge at \mathbf{Q}_{AF} when the energy reaches ~ 50 meV. At higher energies, the scattering disperses outwards, away from \mathbf{Q}_{AF} . At a given energy, the shape of the scattering in the $(h, k, 0)$ zone of reciprocal space forms a square with its corners rotated by 45° relative to the square formed by the low-energy incommensurate wave vectors. Through their \mathbf{Q} dependence, we have been able to identify magnetic excitations up to ~ 200 meV; the scattering strength appears to fall off rapidly above that energy.

3. Similarity to $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

The dispersion of the magnetic excitations described above is extremely similar to new observations on $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ (YBCO6.6) by Hayden *et al.* [6] obtained on the same spectrometer. If one multiplies the energy scale for the features in LBCO by $\sim \frac{2}{3}$ (the approximate ratio of the “resonance” energies) then they match up quite well with those reported for YBCO6.6. Of course, there are certain obvious differences. The YBCO6.6 sample was measured in the superconducting state, whereas LBCO was studied in the normal state. The LBCO has static magnetic order, while the YBCO6.6 has a spin gap of ~ 20 meV. Despite these differences, the similarities suggest that there may be a universal magnetic spectrum common to the hole doped cuprates.

A study of partially detwinned YBCO6.5 by an-

other group, Stock *et al.* [8], confirms the nature of the dispersion. They report that the scattering at high energies forms more of a circle than a square in 2D reciprocal space; however, such discrepancies are of less significance than the universal features that are apparent. A similar dispersion with energy has also been seen in studies of YBCO closer to optimal doping [7,9].

4. Weakly-coupled ladder model

Given that our LBCO sample exhibits stripe order [15], it is natural to look for an explanation of the universal magnetic spectrum in terms of the inhomogeneous antiferromagnetic correlations associated with that order [18,19,20]. Several years ago, Batista, Ortiz, and Balatsky [21] proposed that the magnetic resonance observed in YBCO might be understood in terms of the excitations of an incommensurate spin-density-wave state. They made an analogy with the excitation spectrum observed in (diagonally) stripe-ordered $\text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$ [22,23]. The latter spectrum has since been shown to be well described by linear spin-wave theory [22,24,25,26].

The problem with this picture is that the observed dispersions are different from the predictions of linear spin wave theory applied to ordered stripes, as has been pointed out by Bourges *et al.* [27] in their neutron scattering study of YBCO6.85. Spin waves disperse isotropically from the incommensurate modulation wave vectors, with similar intensities for spin waves dispersing towards and away from the antiferromagnetic wave vector \mathbf{Q}_{AF} . In contrast, there is no sign of any outward dispersing excitations in $\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$, and only dispersion towards \mathbf{Q}_{AF} is seen. Our results for LBCO confirm that the excitations of a stripe-ordered cuprate differ from the predictions of spin-wave theory [5].

Looking at Fig. 1, one can see that, at least in this cartoon version of stripe order, the hole-rich stripes separate 2-leg antiferromagnetic spin ladders. An isolated ladder with superexchange coupling J between nearest-neighbor spins has an excitation gap of $J/2$ [28]. In the ground state the

spins tend to form singlet pairs, and a triplet excitation can propagate along the length of a ladder [29]. We found that the dispersion of an isolated 2-leg ladder with $J = 100$ meV gives a good description of our measurements above 50 meV. Such a model suggests that the gap at the antiferromagnetic wave vector is associated with singlet spin correlations.

To simultaneously describe the incommensurate excitations at lower energies, one must take into account the coupling between the ladders. Calculations of the spectrum under the assumption of weak coupling between the ladders have been reported by Vojta and Ulbricht [30] and by Uhrig, Schmidt, and Grüninger [31]. The former paper was the first to show that the calculated spectrum for weakly-coupled ladders gives a good description of the dispersion in LBCO, while the latter paper included cyclic ring exchange in the ladder Hamiltonian and showed that the model can give quantitative agreement with the absolute scale of the observed magnetic scattering. Some features of the dispersion were anticipated by an earlier calculation by Dalosto and Riera [32]. Good agreement with the measurements is also obtained in a calculation of fluctuations about a mean-field stripe-ordered state by Seibold and Lorenzana [33].

It seems worthwhile to note that there are experimental precedents for the coexistence of quantum excitations with static magnetic order. Such behavior has been seen in compounds containing $S = 1$ spin chains weakly coupled together through magnetic rare-earth ions [34], and in $S = 1$ spin chains doped with holes [35].

5. Fermiology

An alternative approach to the origin of the magnetic excitations in the superconducting cuprates is based on Fermi liquid theory. One calculates the spin susceptibility based on the ability of conduction electrons to scatter across the Fermi surface from filled to empty states [36,37]. From this perspective, the resonance feature is commonly tied to the shape of the electronic Fermi surface and the d -wave nature of the superconducting gap [38,39].

Such calculations are capable of describing (or fitting) features of the observed magnetic excitations, such as incommensurability [40,41,42,43,44,45].

There are various features of this approach that we find to be problematic. There are significant doubts concerning the appropriateness of such calculations in the normal state, especially in the underdoped regime. It is also unclear how to explain charge-stripe order in this picture. (For more discussion of such issues, see Kivelson *et al.* [19].) As our LBCO sample is in the normal state and has charge stripe order, calculations based on fermiology do not seem to be relevant. Given the similarity between the magnetic dispersion in our LBCO sample and that found in YBCO, we question the relevance of fermiology for obtaining a global understanding of the magnetic response in the cuprates.

6. Universal magnetic spectrum and the superconducting spin gap

The LBCO results indicate that the occurrence of commensurate inelastic scattering does not require superconductivity. Thus, what seems to be special about the “resonance” phenomenon is its temperature dependence, and not that the excitation is commensurate. In the superconducting state, the enhanced magnetic signal always appears just above the spin gap. Thus, it appears that one might be able to describe all of the neutron scattering results obtained so far on a variety of hole-doped cuprates with a universal spectral function multiplied by a suitable gap function. The energy scale for the spectrum and the size of the gap are clearly material and doping dependent. Experimentally, the size of the spin gap is roughly correlated with T_c , while the gap at the commensurate wave vector may be an upper limit to the spin gap. Such behavior is consistent with a superconducting mechanism in which spin pairing drives hole pairing [46].

Motivated by mean-field calculations [47], we have calculated a model spin susceptibility based on weakly coupled 2-leg ladders using

$$\chi = \chi_{\text{ladd}} / [1 + J_{\perp} \sin^2(4\pi q_{\perp}) \chi_{\text{ladd}}], \quad (1)$$

where we take

$$\chi_{\text{ladd}} = \frac{1}{\hbar\omega(q_{\parallel})} \cos^2(\pi q_{\parallel}) \cos^2(\pi q_{\perp}) F(\omega), \quad (2)$$

with $\omega(q_{\parallel})$ from [29], and

$$F(\omega) = \frac{1}{E - \hbar\omega(q_{\parallel}) + i\gamma} - \frac{1}{E + \hbar\omega(q_{\parallel}) + i\gamma}, \quad (3)$$

with $q_{\parallel} = h - \frac{1}{2}$, $q_{\perp} = k - \frac{1}{2}$, and $E = \hbar\omega$. Here, J_{\perp} is the effective coupling between ladders, which we set to $0.13J$, where J is the superexchange within a ladder. Figure 2(b) shows the spectrum of χ'' calculated along the path shown in Fig. 2(a), averaged over the two stripe orientations shown in Fig. 1. We take this to be a rough model of the excitation spectrum that we have measured in LBCO.

The major difference between the experimental spectrum for LBCO and that for superconducting cuprates is the spin gap observed below T_c . To model the spin gap, we multiply χ'' by a gap function. We arbitrarily choose to use the BCS gap function, $\text{Re}(E/\sqrt{E^2 - \Delta^2})$, with $\Delta = \Delta_0 + i\Gamma$. The gap function alone is plotted in Fig. 2(c): for $\Gamma = 0.1\Delta_0$ the depression of weight below the gap and the pile up of weight above the gap are apparent, while for $\Gamma = 0.8\Delta_0$ the gap is overdamped. We suggest that the overdamped gap mimics the normal-state response of the doped cuprates.

To mimic optimally and over doped LSCO, we choose $\Delta_0 = 0.1J$, considerably smaller than the ladder gap energy of $0.5J$. The model calculations with overdamped and underdamped gaps are shown in Fig. 2(d) and (e), respectively. Taking these to represent normal state and superconducting responses, we plot the difference in Fig. 2(f), which shows a pile up of weight at incommensurate wave vectors, above a loss of weight at lower energies. The difference, restricted to incommensurate scattering, is similar to experiment [10,12,13]. In contrast, we pick $\Delta_0 = 0.4J$ to mimic YBCO near optimal doping, Fig. 2(g) and (h). The difference, shown in Fig. 2(i), shows a large gain at the commensurate position, with a loss of weight at lower energies, as observed experimentally.

While this comparison is only qualitative, we believe it gives a useful description of experiment. A clear spin gap is only observed in the supercon-

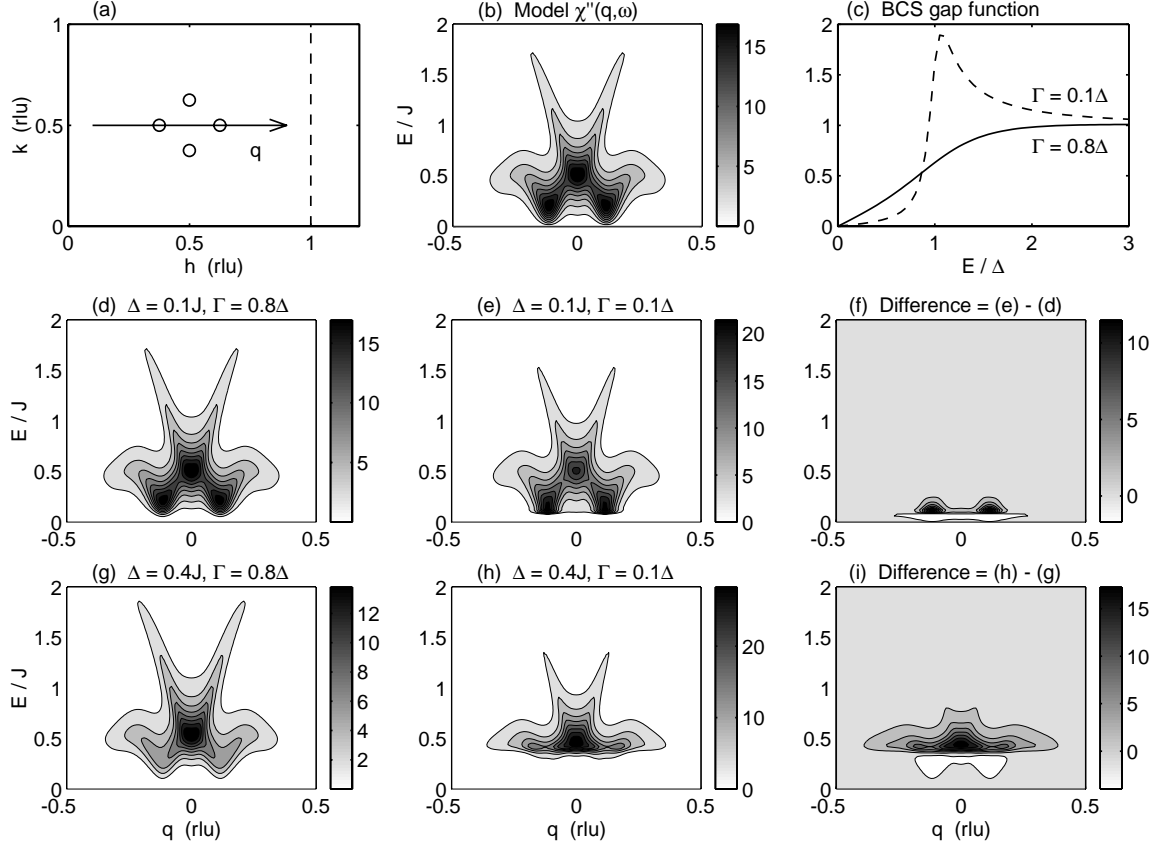


Fig. 2. (a) Arrow indicates path in reciprocal space used in following panels. (b) Model of χ'' as discussed in text. (c) BCS gap function for two choices of Γ . (d) Product of model χ'' and gap function with $\Delta = 0.1(1 + i0.8)J$, and (e) $\Delta = 0.1(1 + i0.1)J$. (f) Difference of (e) and (d). (g) Similar to (d), with $\Delta = 0.4(1 + i0.8)J$, and (h) $\Delta = 0.4(1 + i0.1)J$. (i) Difference of (h) and (g).

ducting state, but an overdamped gap may characterize the normal state, at least in the underdoped regime.

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